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SRA FINAL REPORT

Office of Naval Research Contract: N00014-93-C-0044

TRANSIENT TRANSPORT IN NANOSTRUCTURE DEVICES VIA THE QUANTUM LIOUVILLE EQUATION IN THE COORDINATE REPRESENTATION

Submitted to
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ABSTRACT

Through the use of numerical methods the quantum Liouville equation in the coordinate representation has been implemented for the study of semiconductor devices with nanoscale feature sizes, with an emphasis on dissipation. We have successfully applied this algorithm to the calculation of current in single and multiple barrier diodes, and *Scientific Research Associates, Inc. is presently one of the few research organizations numerically obtaining the quantum distribution functions for both electrons and holes.* This document summarizes work performed under US Navy, Office of Naval Research Contract: N00014-93-C-0044.

1. INTRODUCTION

In the past decade we have seen demonstrations that band structure engineered devices with nanoscale dimensions have the potential of being the basis for a dramatic shift in semiconductor technology. One significant illustration of this has been the development of multiple value logic and memory circuits based on utilization of the negative differential resistance properties of either isolated resonant tunneling structures or embedded RTDs (as in the case of resonant tunneling bipolar transistors).

Generally, the approach to studying these band structured engineered device falls into two categories. *The first category* is concerned with studying fundamental device behavior and predicting device performance through computation of the quantum distribution function. This approach emphasizes the details of transient behavior, the numbers of particles involved in device operation, the temporal duration under which the effective mass approximation is valid, the significance of the Fermi-golden rule, and other short time phenomena. In this approach, when scattering is present, or when time dependent fields are present and treated as perturbations, it is supposed that the perturbation does not modify the states of an unperturbed system, rather the perturbed system instead of remaining permanently in one of the unperturbed states is assumed to be continually changing from one to another, i.e., undergoing transitions from one state to another state. This approach is at the heart of those calculations employing the density matrix, those employing the Wigner distribution function, and those employing Green's function techniques. *The second category*, which is presently, the most popular, obtains solutions to the time independent Schrodinger equation under nonequilibrium conditions, from which the time independent wave functions are obtained. This second procedure does not yield the quantum distribution function, and cannot reliably predict device performance. *The approach taken at Scientific Research Associates, Inc., (SRA), has been to obtain the quantum distribution function as solutions to the density matrix in the coordinate representation.*

This document summarizes ONR Contract N00014-93-C-0044 sponsored studies of the density matrix at SRA.

2. SUMMARY OF STUDIES UNDER ONR CONTRACT N00014-93-C-0044

The density matrix studies at SRA have been developed along very general lines. The SRA code is capable of treating:

- large numbers of particles present in the transport process,
- the effects of the Pauli exclusion principle through boundary conditions,
- electron and hole transport,
- and transients.

The algorithm implemented has deliberately ignored *regional approximations*, where the quantum mechanical region is connected to the classical region via boundary conditions. Instead SRA has obtained the quantum distribution function for the entire structure being studied.

2a. THE ROLE OF DISSIPATION

The structure that we typically dealt with incorporated the specific quantum mechanical barrier/well region and the cladding regions surrounding the barriers. From the outset of the study we incorporated dissipation. This introduces its own set of difficulties. First, as was learned from classical device studies, incorporation of dissipation is essential to any development of a consistent set of device physics. Dissipation is necessary, if current is to flow within the device under steady state conditions. **Dissipation is not required for transient current contributions.** The question we grappled with was what was the best means to incorporate dissipation. Clearly, from an analytical point of view dissipation is best handled by incorporating it in the governing equations.

The simplest form of dissipation is that associated with the relaxation approximation. While questions arise as to whether the relaxation time should be energy dependent, and/or momentum dependent, and/or position dependent, this is the most frequently used approximation. Indeed many of us, who have been involved with classical device transport calculations, routinely incorporated the relaxation time approximation in terms that arose from the *linearized* Boltzmann equation. The linearized Boltzmann equation is often used as the basis for the drift and diffusion equations. But the use of the relaxation time approximation does not deal with one of the most basic of device issues, the representation of the regions between the quantum mechanical barriers and wells, and the physical contacts. It is this region where the carriers undergo sufficient scattering to relax to local steady state values, and result in the concept of a quasi-Fermi level. This problem was dealt with as discussed below.

The presence of a relaxation time in the equation of motion of the density matrix results in a governing equation that is complex, i.e., dissipation introduces an imaginary contribution to the steady state Liouville equation. On the other hand the introduction of a quasi-Fermi energy to the quantum Liouville equation, without regard to a local relaxation time, results in a net change in the local value of the potential energy, ***without an imaginary contribution to the governing equation.*** If these contributions are treated separately, then when using the quasi-Fermi energy approximation, current is introduced through boundary conditions, through, e.g. ***the density matrix equivalent of a displaced Fermi distribution***.

At SRA a wide variety of dissipation models were introduced into the simulations. We implemented the relaxation time approximation but did not emphasize its contribution. Instead we incorporated the concept of the quasi-Fermi energy, whose spatial distribution was determined by the net current, the local carrier density and the ***local*** relaxation time. Current was introduced through the presence of boundary conditions - in the case of solutions to the steady state quantum Liouville equation. We also introduced dissipation through Fokker-Planck contributions. In the case of the density matrix this contribution takes the form:

$$\frac{1}{\tau}\left[\zeta\frac{\partial\rho}{\partial\zeta}+\left(\frac{2\zeta^2}{\lambda^2}\right)\rho\right]$$

Whereas in the case of Wigner transport its form is:

$$-\frac{1}{\tau}\left(\frac{\partial kf}{\partial k}+\frac{1}{\lambda^2}\frac{\partial^2 f}{\partial k^2}\right)$$

The Fokker-Plank terms introduce an imaginary contribution to the Liouville equation in the coordinate representation, and under conditions where the local density is constant the dissipation forces current to flow with parameters varying according to Ohms Law. (The normalizing term in the above equation is the thermal deBroglie wavelength.)

One of the important aspects of this study was an attempt to combine the concept of the quasi-Fermi level and dissipation as expressed through the Fokker-Plank terms. We succeeded in carrying this out for classical systems, and performed several successful numerical simulations. Work was begun on systems containing quantum mechanical elements and simulations were performed for modest quantum mechanical barrier. By the end of this contract period robust quantum mechanical simulations with both Fokker Plank and quasi-Fermi energy contributions were not completed.

The status of the SRA density matrix algorithm at the end of this study is represented by the PI's lecture notes distributed at the NATO ASI on *Quantum Transport in Ultrasmall Devices* (Il Ciocco, Italy, 17-30 July 1994), a copy of which is included with this report. Supplementing the lecture notes were a series of lectures, in which a variety of examples illustrating the effects of *delta doping, the significance of the quantum potential, and initial transient calculations.* Additionally, the study of dissipation, as represented in the SRA algorithm was discussed.

We note that additional discussions of the density matrix and the quantum potential are contained in the following papers, were published:

1. *Modeling of Quantum Transport in Semiconductor Devices,* (with D. K. Ferry) Published by Academic Press, Inc.
2. *Density Matrix Simulations of Semiconductor Devices,* Published by Plenum Press.
3. *Transport in Two-Dimensional Quantum Well HEMTs* (with J. P. Kreskovsky) Proceedings of Third International Conference on Computational Electronics.
4. *Resonant Tunneling Calculations via the Density Matrix in the Coordinate Representation* (with T. R. Govindan) Proceedings of Third International Conference on Computational Electronics.
5. *Electron Transport Using the Quantum Corrected Hydrodynamic Equations* (with J. P. Kreskovsky) Invited paper in *VLSI.*

2b. NON-SELF CONSISTENT TRANSIENT STUDIES

The task associated with the transient calculations was to develop a transient accurate algorithm within the framework of the quantum Liouville equation in the coordinate representations. As in the case of the steady state calculations, the transients were performed along 'characteristic directions'. Thus, much of the effort here was in algorithm development, implementation and testing.

As in most numerical simulations involving transient there are two time intervals to deal with. The first time interval is the physical time interval, the second time interval involves the number of iterations required to get to a converged solution within the prespecified time interval. During the initial stages of the transient algorithm development we focused exclusively on the quantum Liouville equation, ignoring Poisson's equation. We examined both closed and open systems, and calculations were undertaken that *demonstrated the efficacy of the algorithm*. We illustrate the non-self consistent calculations below.

The problem we considered was for a closed system. The initial state of the system consisted of an initial distribution of charge at the left-hand side of the device. While we could have specified an initial charge distribution in the form of a Gaussian – we didn't. Rather we computed a charge distribution from a potential well configuration. The position of the potential well used for the initial charge distribution is displayed in figure 1, where it is represented by the $t < 0$ data. The position of the potential well used in the transient calculation is represented by the $t > 0$ data. This $t > 0$ potential well represents an attractive force on the carriers. The steady state charge distribution arising from this potential well is shown in figure 2, and is represented by the $t = 0$ data points. *We reiterate: the initial potential distribution has no impact on the computations for* $t > 0$. The initial potential distribution is not present at times $t > 0$. It is introduced solely to provide the initial charge distribution.

The initial charge distribution consisted of a buildup of charge at the left side of the structure. Subsequent to this, see figure 2, is a buildup of charge over the right-side quantum well. The structure of the space charge distribution reveals that there are strong nonuniformities in the charge distribution situated around the initial distribution. We know of course, from the discussion of the Bohm quantum potential that there are quantum mechanical forces, whose strength is determined by the **shape** of the carrier distribution. (We note that a similar interpretation can be extracted from calculations where we watch the evolution of a distribution of weighted plane wave states.) The implication of this result is that the **relaxation to steady state** is determined, in part, by **memory of the initial charge distribution.** The physical time sequences are indicated in the figure 2, and we begin to see that the transition to steady state appears to involve a damped oscillation in the charge distribution, **about its initial and final distribution.**

There are two aspects of this calculation that are noteworthy. First is the demonstration that there are memory effects and that these damp out. Second, is the length of the structure used to perform the calculations. The device structure is 200 nm long. Most quantum device simulations are for structures significantly smaller than 200 nm. These cannot separate the quantum mechanical region from the influence of the boundary.

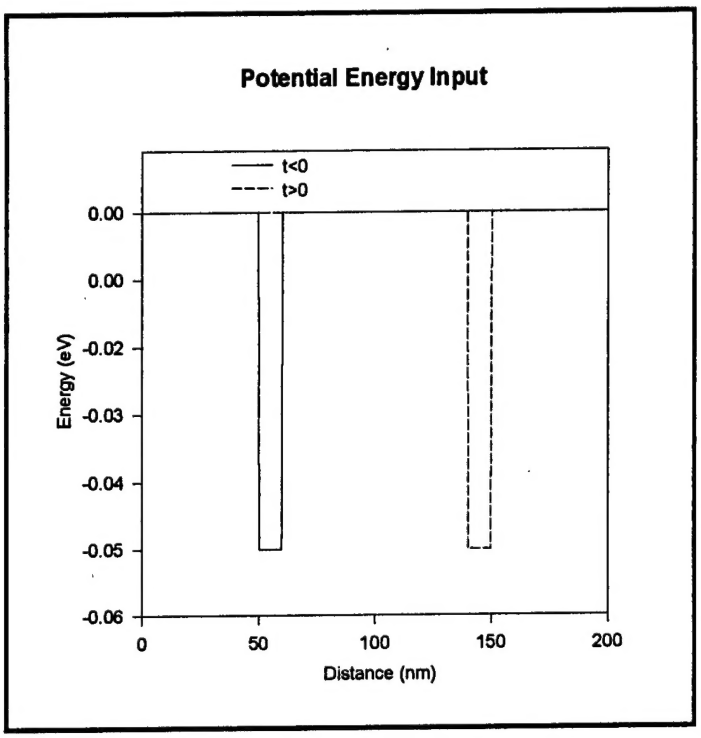

Figure 1. Initial and final states associated with the non-self consistent time dependent calculation.

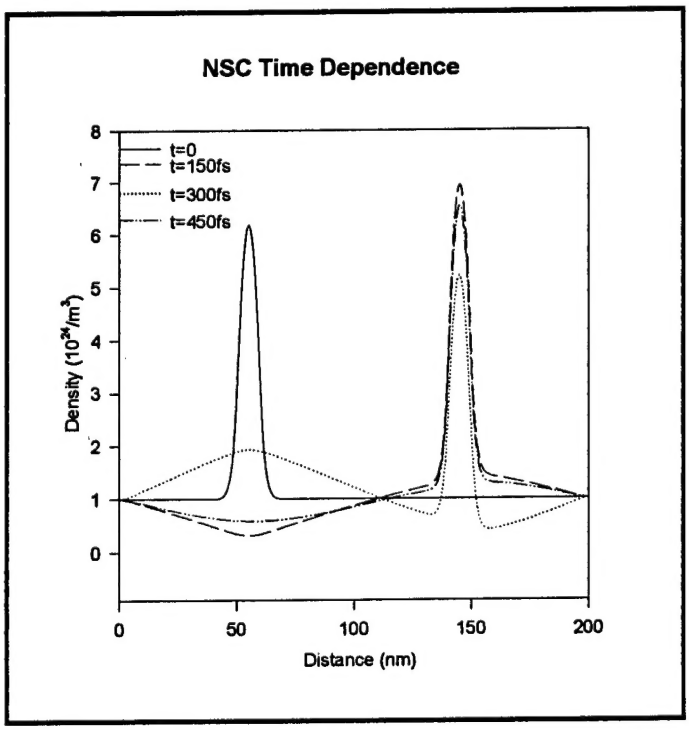

Figure 2. Time dependent distribution of charge associated with the placement of the quantum well to the right hand side of the structure.

2c. SELF-CONSISTENT TRANSIENT STUDIES

At the end of the Contract period we succeeded in demonstrating that the transient self-consistent calculations could be performed. The calculation was performed for a single barrier structure in which a change in bias occurred. *Unlike the non-self consistent studies, these dealt with open boundary conditions in which the time dependent potential, density and current were calculated.*

2d. ANALYTICAL STUDIES

The time dependent density matrix calculations include terms that are consistent with the Fermi golden rule. As such, while they contribute to femtosecond scale transients they do not incorporate the necessary physics associated with short time transient. While subsequent work at SRA in other programs have attempted to generalize dissipation and transients on a short time scale, the work here involved teasing the density matrix algorithm to separate out explicit short time and long time scale events. This was accomplished by submitting the density matrix to second order perturbation theory.

The second order contribution to the *time dependent equation of motion in the coordinate representation is:*

$$<\mathbf{x}|\rho_{op}(t)|\mathbf{x}'>^{(2)}=\int d\mathbf{k}'d\mathbf{x}''d\mathbf{x}'''\left\{\frac{\cos[\omega(\mathbf{k}+\mathbf{q},\mathbf{k})+\omega_o](t_0-t)-1}{[\hbar\omega(\mathbf{k}+\mathbf{q},\mathbf{k})+\hbar\omega_o]^2}\right\}|M(\mathbf{k},\mathbf{k}-\mathbf{q})|^2$$

$$X\left\{\begin{array}{l}\left\{\begin{array}{l}<\mathbf{x}|\mathbf{k}><\mathbf{k}|\mathbf{x}''><\mathbf{x}''|\rho_{op}(t)|\mathbf{x}'''>^{(0)}<\mathbf{x}'''|\mathbf{x}'> \\ \quad -<\mathbf{x}|\mathbf{k}+\mathbf{q}><\mathbf{k}|\mathbf{x}''><\mathbf{x}''|\rho_{op}(t)|\mathbf{x}'''>^{(0)}<\mathbf{x}'''|\mathbf{k}><\mathbf{k}+\mathbf{q}|\mathbf{x}'>\end{array}\right\} \\ +\left\{\begin{array}{l}<\mathbf{x}|\mathbf{x}''><\mathbf{x}''|\rho_{op}(t)|\mathbf{x}'''>^{(0)}<\mathbf{x}'''|\mathbf{k}><\mathbf{k}|\mathbf{x}'> \\ \quad -<\mathbf{x}|\mathbf{k}+\mathbf{q}><\mathbf{k}|\mathbf{x}''><\mathbf{x}''|\rho_{op}(t)|\mathbf{x}'''>^{(0)}<\mathbf{x}'''|\mathbf{k}><\mathbf{k}+\mathbf{q}|\mathbf{x}'>\end{array}\right\}\end{array}\right\} \quad (1)$$

In the above expression the term $|M(\mathbf{k},\mathbf{k}-\mathbf{q})|^2$ represents the square of the matrix element associated with the perturbation, and the second contribution in the large curly brackets represents differences in the zeroth order density matrix between different quantum states. As a sanity check we note that in the long time limit the above expression yields standard perturbation theory with the Fermi golden rule.

More generally after performing, formally, the necessary time integrations, the density matrix to second order in perturbation theory provides the following:

$$
-\left[\frac{1}{\hbar^2}\right]\left[\begin{array}{l}
\int_{t_0}^{t} d\tau \int_{t_0}^{\tau} d\tau' \int \langle \mathbf{x}|\mathbf{k}\rangle d\mathbf{k}\left[e^{i\omega(\mathbf{k},\mathbf{k}')(\tau-t)}\langle \mathbf{k}|\begin{Bmatrix}\delta V_1(\mathbf{q})e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau)}\\ +\delta V_2(\mathbf{q})e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau)}\end{Bmatrix}|\mathbf{k}'\rangle d\mathbf{k}'\right.\\
\left. X\ e^{i\omega(\mathbf{k}',\mathbf{k}'')(\tau'-t)}\langle \mathbf{k}'|\begin{Bmatrix}\delta V_1(\mathbf{q})e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau')}\\ +\delta V_2(\mathbf{q})e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau')}\end{Bmatrix}|\mathbf{k}''\rangle\right]\\
\qquad X\, d\mathbf{k}''\langle \mathbf{k}''|\mathbf{x}''\rangle d\mathbf{x}''\langle \mathbf{x}''|\rho_{op}(t)|\mathbf{x}'\rangle^{(0)}\\
+\int\langle \mathbf{x}|\rho_{op}(t)|\mathbf{x}''\rangle^{(0)}\, d\mathbf{x}''\int_{t_0}^{t} d\tau\int_{t_0}^{t} d\tau'\int \langle \mathbf{x}''|\mathbf{k}\rangle d\mathbf{k}\\
\qquad X\left[e^{i\omega(\mathbf{k},\mathbf{k}')(\tau'-t)}\langle \mathbf{k}|\begin{Bmatrix}\delta V_1(\mathbf{q})e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau')}\\ +\delta V_2(\mathbf{q})e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau')}\end{Bmatrix}|\mathbf{k}'\rangle d\mathbf{k}'\right.\\
\qquad \left. X\ e^{i\omega(\mathbf{k}',\mathbf{k}'')(\tau-t)}\langle \mathbf{k}'|\begin{Bmatrix}\delta V_1(\mathbf{q})e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau)}\\ +\delta V_2(\mathbf{q})e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau)}\end{Bmatrix}|\mathbf{k}''\rangle\right] d\mathbf{k}''\langle \mathbf{k}''|\mathbf{x}'\rangle\\
-\int_{t_0}^{t} d\tau\int \langle \mathbf{x}|\mathbf{k}\rangle d\mathbf{k}\left[e^{i\omega(\mathbf{k},\mathbf{k}')(\tau-t)}\langle \mathbf{k}|\begin{Bmatrix}\delta V_1(\mathbf{q})e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau)}\\ +\delta V_2(\mathbf{q})e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau)}\end{Bmatrix}|\mathbf{k}'\rangle\right]\\
\qquad X\ d\mathbf{k}'\langle \mathbf{k}'|\mathbf{x}''\rangle d\mathbf{x}''\langle \mathbf{x}''|\rho_{op}(t)|\mathbf{x}'''\rangle^{(0)}\, d\mathbf{x}'''\int_{t_0}^{t} d\tau'\int \langle \mathbf{x}'''|\mathbf{k}''\rangle d\mathbf{k}''\\
\qquad X\left[e^{i\omega(\mathbf{k}'',\mathbf{k}''')(\tau'-t)}\langle \mathbf{k}''|\begin{Bmatrix}\delta V_1(\mathbf{q})e^{i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau')}\\ +\delta V_2(\mathbf{q})e^{-i(\mathbf{q}\cdot\mathbf{r}-\omega_o\tau')}\end{Bmatrix}|\mathbf{k}'''\rangle\right] d\mathbf{k}'''\langle \mathbf{k}'''|\mathbf{x}'\rangle
\end{array}\right] \tag{2}
$$

The above equation is not very transparent, but if we perform the indicated time integration, the first two contributions provide an indication of the early time transients, which are shown in equation (3). Equation (3) indicates that an expansion of the exponential contribution will yield and early time contribution that is of order $(t-t_0)^2$. **The significance of this result is that it indicates that it may be possible to break up the scattering contribution into explicit short time and long time contributions.**

$$
\left[\int d\mathbf{k} d\mathbf{x}'' \left[\left\{ \frac{t_0 - t}{i\hbar^2[\omega(\mathbf{k}-\mathbf{q},\mathbf{k}) + \omega_o]} + \frac{e^{i[\omega(\mathbf{k}-\mathbf{q},\mathbf{k})+\omega_o](t_0-t)} - 1}{[\hbar\omega(\mathbf{k}-\mathbf{q},\mathbf{k}) + \hbar\omega_o]^2} \right\} I_1(\mathbf{k},\mathbf{k}-\mathbf{q}) I_2(\mathbf{k}-\mathbf{q},\mathbf{k}) \right.\right.
$$

$$
\left.\left. + \left\{ \frac{t_0 - t}{i\hbar^2[\omega(\mathbf{k}+\mathbf{q},\mathbf{k}) - \omega_o]} + \frac{e^{i[\omega(\mathbf{k}+\mathbf{q},\mathbf{k})-\omega_o](t_0-t)} - 1}{[\hbar\omega(\mathbf{k}+\mathbf{q},\mathbf{k}) - \hbar\omega_o]^2} \right\} I_2(\mathbf{k},\mathbf{k}+\mathbf{q}) I_1(\mathbf{k}+\mathbf{q},\mathbf{k}) \right] \right.
$$

$$
\times <\mathbf{x}|\mathbf{k}><\mathbf{k}|\mathbf{x}''><\mathbf{x}''|\rho_{op}(t)|\mathbf{x}'>^{(0)}
$$

(3)

$$
\left. \int <\mathbf{x}|\rho_{op}(t)|\mathbf{x}''>^{(0)} d\mathbf{x}'' \int d\mathbf{k} \left[\left\{ \frac{t_0 - t}{i\hbar^2[\omega(\mathbf{k},\mathbf{k}-\mathbf{q}) - \omega_o]} + \frac{e^{i[\omega(\mathbf{k},\mathbf{k}-\mathbf{q})-\omega_o](t_0-t)} - 1}{[\hbar\omega(\mathbf{k},\mathbf{k}-\mathbf{q}) - \hbar\omega_o]^2} \right\} I_1(\mathbf{k},\mathbf{k}-\mathbf{q}) I_2(\mathbf{k}-\mathbf{q},\mathbf{k}) \right.\right.
$$

$$
\left.\left. + \left\{ \frac{t_0 - t}{i\hbar^2[\omega(\mathbf{k},\mathbf{k}+\mathbf{q}) - \omega_o]} + \frac{e^{i[\omega(\mathbf{k},\mathbf{k}+\mathbf{q})-\omega_o](t_0-t)} - 1}{[\hbar\omega(\mathbf{k},\mathbf{k}+\mathbf{q}) - \hbar\omega_o]^2} \right\} I_2(\mathbf{k},\mathbf{k}+\mathbf{q}) I_1(\mathbf{k}+\mathbf{q},\mathbf{k}) \right] \right]
$$

$$
\times <\mathbf{x}''|\mathbf{k}><\mathbf{k}|\mathbf{x}'>
$$

3. SUMMARY AND COMMENTS ON RECENT STUDIES

The discussion of the previous sections summarizes the work completed under Contract N00014-93-C-0044. What are some of the issues that are germane to this study that have transpired since this study was completed?

First, the spate of device simulations utilizing either the density matrix in the coordinate representation or the Wigner function analysis have provided us with demonstrations of what these simulations can do. **But these simulations have not been used for detailed device design, and this is a source of disappointment.** (The closest attempt at a combined theory and experiment study has been that of the NEMO team, but their study has not produced a transient analysis and there are other issues to be dealt with as we discuss below.) Indeed, with the exception of the density matrix in the coordinate representation, undertaken by workers at SRA, no other quantum device simulation has reproduced Ohms law!

Analyzing the different approaches of these device simulations, in particular the Wigner simulations, indicates both physics and numerical based deficiencies. The latter is associated with

the number of grid points used for the study, the size of the device simulated, and the algorithm used to convert the governing partial differential equation to the required difference equation.

What are some of the physics based issues particularly as they affect device physics and dissipation? As discussed above the ones of interest include the role of dissipation. We know from classical physics that a solution to the collisionless Boltzmann equation does not yield a finite steady dc current, although there can be a transient current. Similarly the collisionless Wigner equation does not yield a steady dc current, only a transient current without the incorporation of dissipation in the governing equation.

We point out that advances in classical device simulation, which include Gunn devices, IMPATTs, HBTs, FETs, do not treat current as a boundary condition---it is an integral part of the simulation. Thus when we see published papers of simulations with and without scattering we need to ask what they signify and how they can be performed properly. The suggestion for a suitable approach is as follows: The device simulated should consist *conceptually*, of three distinct regions: two boundary regions probably each 50nm to 100nm long surrounding the third region containing the quantum structure. The boundary regions should be **dissipative**, as they would be in an actual structure. The quantum mechanical region can initially be modeled ignoring scattering assuming that all transport is ballistic. Then for comparison, scattering is introduced into the quantum mechanical region.

The heart of the matter is this: ***after the quantum mechanical nature of device transport is established the role of dissipation must be explicitly incorporated into the analysis.***